An Introduction to Support Vector Machine

> MAP i - Computer Vision 2011/12 Jaime S. Cardoso INESC Porto, Faculdade Engenharia, Universidade do Porto 2012/01/02

# What is pattern recognition?

"The assignment of a physical object or event to one of several prespecified categories" -- Duda & Hart

- A pattern is an object, process or event that can be given a name.
- A pattern class (or category) is a set of patterns sharing common attributes and usually originating from the same source.
- During recognition (or classification) given objects are assigned to prescribed classes.
- A **classifier** is a machine which performs classification.



# Basic concepts



Feature vector  $\mathbf{x} \in X$ 

- A vector of observations (measurements).

-  $\mathbf{x}$  is a point in feature space X.

Hidden state

 $y \in Y$ 

- Cannot be directly measured.

- Patterns with equal hidden state belong to the same class.

#### <u>Task</u>

- To design a classifer (decision rule)  $q: X \rightarrow Y$ 

which decides about a hidden state based on an onbservation.





Task: jockey-hoopster recognition.

The set of hidden state is  $Y = \{H, J\}$ The feature space is  $X = \Re^2$ 

<u>Training examples</u>  $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_l, y_l)\}$ 

Linear classifier:

$$\mathbf{q}(\mathbf{x}) = \begin{cases} H & if \quad (\mathbf{w} \cdot \mathbf{x}) + b \ge 0\\ J & if \quad (\mathbf{w} \cdot \mathbf{x}) + b < 0 \end{cases}$$

# Components of PR system



- Sensors and preprocessing.
- A feature extraction aims to create discriminative features good for classification.
- A classifier.
- A teacher provides information about hidden state -- supervised learning.
- A learning algorithm sets PR from training examples.

#### Feature extraction

Task: to extract features which are good for classification.

Good features: • Objects from the same class have similar feature values.

• Objects from different classes have different values.



### Feature extraction methods



Problem can be expressed as optimization of parameters of feature extractor  $\phi(\theta)$ 

**Supervised methods**: objective function is a criterion of separability (discriminability) of labeled examples, e.g., linear discriminat analysis (LDA).

**Unsupervised methods**: lower dimensional representation which preserves important characteristics of input data is sought for, e.g., principal component analysis (PCA).

# Classifier

A classifier partitions feature space X into **class-labeled regions** such that

 $X=X_1\cup X_2\cup\ldots\cup X_{|Y|}\quad\text{and}\quad X_1\cap X_2\cap\ldots\cap X_{|Y|}=\{0\}$ 



The classification consists of determining to which region a feature vector **x** belongs to.

Borders between decision boundaries are called decision regions.

### Representation of classifier

A classifier is typically represented as a set of discriminant functions

$$\mathbf{f}_i(\mathbf{x}): X \to \mathfrak{R}, i = 1, \dots, |Y|$$

The classifier assigns a feature vector **x** to the *i*-the



**Discriminant function** 

# Review: What We've Learned So Far

- Bayesian Decision Theory
- Maximum-Likelihood & Bayesian Parameter Estimation
- Parametric Density Estimation
- Nonparametric Density Estimation
  - Parzen-Window,  $k_n$ -Nearest-Neighbor

- K-Nearest Neighbor Classifier
- Decision Tree Classifier

# Today: Support Vector Machine (SVM)

- A classifier derived from statistical learning theory by Vapnik, et al. in 1992
- SVM became famous when, using images as input, it gave accuracy comparable to neural-network with hand-designed features in a handwriting recognition task
- Currently, SVM is widely used in object detection & recognition, content-based image retrieval, text recognition, biometrics, speech recognition, etc.
- Also used for regression (will not cover today)



# Outline

- Linear Discriminant Function
- Large Margin Linear Classifier
- Nonlinear SVM: The Kernel Trick
- Demo of SVM

#### **Slides from Jinwei Gu**

#### Discriminant Function

It can be arbitrary functions of x, such as:



g(x) is a linear function:

 $g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$ 

 A hyper-plane in the feature space



**n** =



 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



denotes +1

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!



#### Linear Discriminant Function denotes +1 denotes -1 How would you classify $X_2$ these points using a linear discriminant function in order to minimize the error rate? Infinite number of answers! X<sub>1</sub>

 How would you classify these points using a linear discriminant function in order to minimize the error rate?

Infinite number of answers!

Which one is the best?

X<sub>1</sub>

denotes +1

denotes -1

- The linear discriminant function (classifier) with the maximum margin is the best
- Margin is defined as the width that the boundary could be increased by before hitting a data point
- Why it is the best?
  - Robust to outliners and thus strong generalization ability



Given a set of data points:  $\{(\mathbf{x}_i, y_i)\}, i = 1, 2, \dots, n, \text{ where}$ For  $y_i = +1$ ,  $\mathbf{w}^T \mathbf{x}_i + b > 0$ 

For 
$$y_i = -1$$
,  $\mathbf{w}^T \mathbf{x}_i + b < 0$ 

With a scale transformation on both w and b, the above is equivalent to

For 
$$y_i = +1$$
,  $\mathbf{w}^T \mathbf{x}_i + b \ge 1$ 

For  $y_i = -1$ ,  $\mathbf{w}^T \mathbf{x}_i + b \le -1^{-1}$ 



denotes +1









Quadratic programming with linear constraints

minimize 
$$\frac{1}{2} \| \mathbf{w} \|^2$$
  
s.t.  $y_i (\mathbf{w}^T \mathbf{x}_i + b) \ge 1$ 

Lagrangian Function

minimize 
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left( y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$
  
s.t.  $\alpha_i \ge 0$ 

minimize 
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left( y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$
  
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minimize 
$$L_p(\mathbf{w}, b, \alpha_i) = \frac{1}{2} \|\mathbf{w}\|^2 - \sum_{i=1}^n \alpha_i \left( y_i(\mathbf{w}^T \mathbf{x}_i + b) - 1 \right)$$
  
s.t.  $\alpha_i \ge 0$ 

Lagrangian Dual Problem

$$\begin{array}{ll} \text{maximize} & \sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} \mathbf{x}_{i}^{T} \mathbf{x}_{j} \\ \text{s.t.} & \alpha_{i} \geq 0 \text{ , and } & \sum_{i=1}^{n} \alpha_{i} y_{i} = 0 \end{array}$$

From KKT condition, we know:

$$\alpha_i \left( y_i (\mathbf{w}^T \mathbf{x}_i + b) - 1 \right) = 0$$

- Thus, only support vectors have  $\alpha_i \neq 0$
- The solution has the form:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_{i} y_{i} \mathbf{x}_{i} = \sum_{i \in \mathrm{SV}} \alpha_{i} y_{i} \mathbf{x}_{i}$$

get *b* from 
$$y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1 = 0$$
,  
where **x** is support vector

where  $\mathbf{A}_i$  is support



The linear discriminant function is:

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b = \sum_{i \in SV} \alpha_i \mathbf{x}_i^T \mathbf{x} + b$$

- Notice it relies on a *dot product* between the test point *x* and the support vectors *x<sub>i</sub>*
- Also keep in mind that solving the optimization problem involved computing the dot products x<sub>i</sub><sup>T</sup>x<sub>j</sub> between all pairs of training points

 What if data is not linear separable? (noisy data, outliers, etc.)

 Slack variables ξ<sub>i</sub> can be added to allow misclassification of difficult or noisy data points



Formulation:

minimize 
$$\frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$$

such that

$$y_i(\mathbf{w}^T\mathbf{x}_i+b) \ge 1 - \xi_i$$
$$\xi_i \ge 0$$

Parameter C can be viewed as a way to control over-fitting.

Formulation: (Lagrangian Dual Problem)

maximize 
$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

such that

$$0 \le \alpha_i \le C$$
$$\sum_{i=1}^n \alpha_i y_i = 0$$

## Non-linear SVMs

Datasets that are linearly separable with noise work out great:



But what are we going to do if the dataset is just too hard?



How about... mapping data to a higher-dimensional space:



This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm\_tutorial.ppt

# Non-linear SVMs: Feature Space

 General idea: the original input space can be mapped to some higher-dimensional feature space where the training set is separable:



#### Nonlinear SVMs: The Kernel Trick

• With this mapping, our discriminant function is now:

$$g(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b = \sum_{i \in SV} \alpha_i \phi(\mathbf{x}_i)^T \phi(\mathbf{x}) + b$$

- No need to know this mapping explicitly, because we only use the dot product of feature vectors in both the training and test.
- A kernel function is defined as a function that corresponds to a dot product of two feature vectors in some expanded feature space:

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$
### Nonlinear SVMs: The Kernel Trick

An example:

2-dimensional vectors  $\mathbf{x} = [x_1 \ x_2];$ 

let  $K(x_i, x_j) = (1 + x_i^T x_j)^2$ ,

Need to show that  $K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$ :

$$\begin{split} K(\mathbf{x_{i}}, \mathbf{x_{j}}) &= (1 + \mathbf{x_{i}}^{\mathrm{T}} \mathbf{x_{j}})^{2}, \\ &= 1 + x_{iI}^{2} x_{jI}^{2} + 2 x_{iI} x_{jI} x_{i2} x_{j2} + x_{i2}^{2} x_{j2}^{2} + 2 x_{iI} x_{jI} + 2 x_{i2} x_{j2} \\ &= [1 \ x_{iI}^{2} \ \sqrt{2} \ x_{iI} x_{i2} \ x_{i2}^{2} \ \sqrt{2} x_{iI} \ \sqrt{2} x_{i2}]^{\mathrm{T}} [1 \ x_{jI}^{2} \ \sqrt{2} \ x_{jI} x_{j2} \ x_{j2}^{2} \ \sqrt{2} x_{j1} \ \sqrt{2} x_{j2}] \\ &= \varphi(\mathbf{x_{i}})^{\mathrm{T}} \varphi(\mathbf{x_{j}}), \quad \text{where } \varphi(\mathbf{x}) = [1 \ x_{I}^{2} \ \sqrt{2} \ x_{I} x_{2} \ x_{2}^{2} \ \sqrt{2} x_{I} \ \sqrt{2} x_{2}] \end{split}$$

This slide is courtesy of www.iro.umontreal.ca/~pift6080/documents/papers/svm\_tutorial.ppt

#### Nonlinear SVMs: The Kernel Trick

- Examples of commonly-used kernel functions:
  - Linear kernel:  $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
  - Polynomial kernel:  $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$
  - Gaussian (Radial-Basis Function (RBF)) kernel:  $K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2})$
  - Sigmoid:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$$

 In general, functions that satisfy *Mercer's condition* can be kernel functions.

# Nonlinear SVM: Optimization

Formulation: (Lagrangian Dual Problem)

maximize 
$$\sum_{i=1}^{n} \alpha_{i} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i} \alpha_{j} y_{i} y_{j} K(\mathbf{x}_{i}, \mathbf{x}_{j})$$
such that 
$$0 \le \alpha_{i} \le C$$
$$\sum_{i=1}^{n} \alpha_{i} y_{i} = 0$$

The solution of the discriminant function is

$$g(\mathbf{x}) = \sum_{i \in \mathrm{SV}} \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b$$

The optimization technique is the same.

# Support Vector Machine: Algorithm

- 1. Choose a kernel function
- 2. Choose a value for C
- 3. Solve the quadratic programming problem (many software packages available)
- 4. Construct the discriminant function from the support vectors

#### Some Issues

#### Choice of kernel

- Gaussian or polynomial kernel is default
- if ineffective, more elaborate kernels are needed

- domain experts can give assistance in formulating appropriate similarity measures

#### Choice of kernel parameters

- e.g.  $\sigma$  in Gaussian kernel
- $\sigma$  is the distance between closest points with different classifications
- In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.
- Optimization criterion Hard margin v.s. Soft margin
  - a lengthy series of experiments in which various parameters are tested

# Summary: Support Vector Machine

#### 1. Large Margin Classifier

Better generalization ability & less over-fitting

#### 2. The Kernel Trick

- Map data points to higher dimensional space in order to make them linearly separable.
- Since only dot product is used, we do not need to represent the mapping explicitly.

## Additional Resource

- <u>http://www.kernel-machines.org/</u>
- <u>http://www.csie.ntu.edu.tw/~cjlin/libsvm/</u>

## Multiclass classification

#### Reduction techniques

- Conventional approaches
  - One-against-All
    - K two-class problems
  - Pairwise
    - □ K(K 1)/2 two-class problems
  - Decision-Tree-Based
  - DAG (Directed Acyclic Graph)
  - Error-Correcting Output Codes

## Multiclass classification

#### Reduction techniques

Conventional approaches

- apply binary classifier 1 to test example and get prediction F1 (0/1)
- apply binary classifier 2 to test example and get prediction F2 (0/1)

**...** 

- apply binary classifier M to test example and get prediction FM (0/1)
- use all M classifications to get the final multiclass classification 1..K

#### Feature extraction methods



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# Artificial Neural Networks

Slides from Andrew L. Nelson and Torsten Reil

## What are Neural Networks?

- Models of the brain and nervous system
- Highly parallel
  - Process information much more like the brain than a serial computer
- Learning
- Very simple principles
- Very complex behaviours
- Applications
  - As powerful problem solvers
  - As biological models

# Biologically Inspired

- Electro-chemical signals
- Threshold output firing



# The Perceptron

- Binary classifier functions
- Threshold activation function



The Perceptron: Threshold Activation Function

- Binary classifier functions
- Threshold activation function



Nonlinear Activation Functions

#### Sigmoid Neuron unit function



Linear Activation functions

Output is scaled sum of inputs



## ANNs – The basics

ANNs incorporate the two fundamental components of biological neural nets:

- 1. Neurones (nodes)
- 2. Synapses (weights)



#### Feed-forward nets



#### Feeding data through the net:

Input

Output



Hidden

# $(1 \times 0.25) + (0.5 \times (-1.5)) = 0.25 + (-0.75) = -0.5$

Squashing: 
$$\frac{1}{1+e^{0.5}} = 0.3775$$

 Data is presented to the network in the form of activations in the input layer

#### Examples

- Pixel intensity (for pictures)
- Molecule concentrations (for artificial nose)
- Share prices (for stock market prediction)
- Data usually requires preprocessing
  - Analogous to senses in biology
- How to represent more abstract data, e.g. a name?
  - Choose a pattern, e.g.
    - 0-0-1 for "Chris"
    - 0-1-0 for "Becky"

 Weight settings determine the behaviour of a network

 $\rightarrow$  How can we find the right weights?

#### **Training the Network - Learning**

- Backpropagation
  - Requires training set (input / output pairs)
  - Starts with small random weights
  - Error is used to adjust weights (supervised learning)
  - $\rightarrow$  Gradient descent on error landscape



### Training Data Set

Adjust weights (w) to learn a given target function: y = f(x)

Given a set of training data  $X \rightarrow Y$ 



Training Weights: Error Back-Propagation (BP)

Weight update formula:

$$w(k+1) = w(k) + \Delta w$$

$$\Delta w(i) = \eta * \frac{\partial e(i)}{\partial w}$$

## Error Back-Propagation (BP)













$$\frac{\partial u_{out,1}}{\partial y_{hid}} = \frac{\partial}{\partial y_{hid}} W_{out,1} y_{hid,1}$$
$$= W_{out,1}$$





$$\frac{\partial e}{\partial w_{hid}} = \frac{\partial u_{hid,1}}{\partial w_{hid,1}} \frac{\partial y_{hid}}{\partial u_{hid,1}} \frac{\partial u_{out,1}}{\partial y_{hid}} \frac{\partial y_{out}}{\partial u_{out,1}} \frac{\partial e}{\partial y_{out}}$$
$$= (x) \Big( y_{hid} (u_{hid,1}) \Big[ 1 - y_{hid} (u_{hid,1}) \Big] \Big) (w_{out,1}) (1) (y_{out} - y_{train}) \Big]$$



$$= (y_{hid})(1)(y_{out} - y_{train})$$
- Single hidden layer: 3 Sigmoid neurons
- 2 inputs, 1 output

	x1	x2	у
Example 1	0	0	0
Example 2	0	1	1
Example 3	1	0	1
Example 4	1	1	0

Desired I/O table (XOR):

#### Training error over epoch



initial\_weights = 0.0654 0.2017 0.0769 0.1782 0.0243 0.0806 0.0174 0.1270 0.0599 0.1184 0.1335 0.0737 0.1511

final\_weights = 4.6970 -4.6585 2.0932 5.5168 -5.7073 -3.2338 -0.1886 1.6164 -0.1929 -6.8066 6.8477 -1.6886 4.1531

Mapping produced by the trained neural net:

	x1	x2	У
Example 1	0	0	0.0824
Example 2	0	1	0.9095
Example 3	1	0	0.9470
Example 4	1	1	0.0464

#### Example: Overtraining

- Single hidden layer: 10
  Sigmoid neurons
- 1 input, 1 output



#### **Applications of Feed-forward nets**

- Pattern recognition
  - <u>Character recognition</u>
  - Face Recognition
- Sonar mine/rock recognition (Gorman & Sejnowksi, 1988)
- Navigation of a car (Pomerleau, 1989)
- Stock-market prediction
- Pronunciation (NETtalk)

(Sejnowksi & Rosenberg, 1987)